Welcome to STN International! Enter x:x

LOGINID: ssptansc1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
                Web Page for STN Seminar Schedule - N. America
NEWS
NEWS
        MAR 15
                WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS
     3 MAR 16 CASREACT coverage extended
NEWS
     4 MAR 20 MARPAT now updated daily
NEWS
        MAR 22 LWPI reloaded
NEWS
     6 MAR 30 RDISCLOSURE reloaded with enhancements
     7
NEWS
        APR 02
                JICST-EPLUS removed from database clusters and STN
        APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS
     8
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 10 APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 11 APR 30
                INPADOC replaced by INPADOCDB on STN
NEWS 12 MAY 01
                New CAS web site launched
NEWS 13 MAY 08
                CA/CAplus Indian patent publication number format defined
NEWS 14
        MAY 14
                RDISCLOSURE on STN Easy enhanced with new search and display
                 fields
NEWS 15 MAY 21
                BIOSIS reloaded and enhanced with archival data
NEWS 16 MAY 21
                TOXCENTER enhanced with BIOSIS reload
NEWS 17 MAY 21
                CA/CAplus enhanced with additional kind codes for German
                patents
NEWS 18 MAY 22
                CA/CAplus enhanced with IPC reclassification in Japanese
NEWS 19
        JUN 27
                CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20 JUN 29
                STN Viewer now available
NEWS 21 JUN 29
                STN Express, Version 8.2, now available
NEWS 22 JUL 02
                LEMBASE coverage updated
NEWS 23 JUL 02
                LMEDLINE coverage updated
NEWS 24
        JUL 02
                SCISEARCH enhanced with complete author names
NEWS 25
         JUL 02
                CHEMCATS accession numbers revised
        JUL 02
NEWS 26
                CA/CAplus enhanced with utility model patents from China
NEWS EXPRESS
             29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2;
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS LOGIN
              Welcome Banner and News Items
              For general information regarding STN implementation of IPC 8
```

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 09:45:20 ON 12 JUL 2007

=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE

TOŤAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 09:45:44 ON 12 JUL 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4 DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10612240.str

chain nodes: 18 24 25 26

18 24 25 26 27 28 29 30 31

ring nodes :

 $1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 10 \quad 11 \quad 12 \quad 13 \quad 14 \quad 15 \quad 16 \quad 17 \quad 19 \quad 20 \quad 21 \quad 22 \quad 23$

chain bonds :

7-18 10-17 13-24 18-28 20-26 21-25 22-27 28-29 28-30 30-31

ring bonds :

1-2 1-6 2-3 2-14 3-4 3-16 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-13

11-12 12-13 14-15 15-16 17-19 17-23 19-20 20-21 21-22 22-23

exact/norm bonds :

2-14 3-16 5-7 6-10 7-8 7-18 8-9 8-11 9-10 9-13 10-17 11-12 12-13 13-24

14-15 15-16 18-28 28-29 30-31

exact bonds :

20-26 21-25 22-27 28-30

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 17-19 \quad 17 \div 23 \quad 19-20 \quad 20-21 \quad 21-22 \quad 22-23$

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STF

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> S L1 SSS SAM

SAMPLE SEARCH INITIATED 09:46:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 51 TO ITERATE

100.0% PROCESSED

51 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

592 TO 1448

PROJECTED ANSWERS:

6 TO 266

L2

6 SEA SSS SAM L1

=> D SCAN

L2 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Pyrrole-3-carboxylic acid, 2,5-dihydro-1-hydroxy-2,2,5,5-tetramethyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-

trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)

MF C31 H35 N O10

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

Me Me

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2-Pyridinecarboxylic acid, 5-butyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]1,3-dioxol-5-yl ester (9CI)

MF C32 H33 N O9

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

Оме

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Indole-3-acetic acid, 1-methyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]1,3-dioxol-5-yl ester (9CI)

MF C33 H31 N O9

Absolute stereochemistry.

PAGE 2-A

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FIL CAPLUS COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.90

1.11

FILE 'CAPLUS' ENTERED AT 09:47:09 ON 12 JUL 2007
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FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3 FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.

They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> E US2003-612240/APPS
             2
                   US2003-612233/AP
             5
E2
                   US2003-612237/AP
E3
             1 --> US2003-612240/AP
E4
                   US2003-612240/PRN
             1
E5
             3
                   US2003-612241/AP
E6
             3
                   US2003-612241/PRN
E7
                   US2003-612242/AP
             1
E8
             1
                   US2003-612243/AP
E9
             1
                US2003-612243/PRN
E10
             5
                   US2003-612244/AP
E11
             1
                   US2003-612252/AP
E12
                   US2003-612252/PRN
=> S E3
L3
             1 US2003-612240/AP
```

=> SEL RN L3

E1 THROUGH E52 ASSIGNED

=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 3.03 4.14

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:48:20 ON 12 JUL 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

```
=> S E1-E52

1 108-30-5/BI

(108-30-5/RN)

1 132-60-5/BI

(132-60-5/RN)

1 151838-62-9/BI
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1 15761-39-4/BI
    (15761-39-4/RN)
1 171047-77-1/BI
    (171047-77-1/RN)
1 176446-74-5/BI
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1 1877-75-4/BI
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1 1878-91-7/BI
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1 1878-94-0/BI
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1 22042-71-3/BI
    (22042-71-3/RN)
1 28547-08-2/BI
    (28547-08-2/RN)
1 305-03-3/BI
    (305-03-3/RN)
1 401478-57-7/BI
    (401478-57-7/RN)
1 405-79-8/BI
    (405-79-8/RN)
1 47789-93-5/BI
    (47789-93-5/RN)
1 4940-39-0/BI
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1 499-81-0/BI
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1 518-28-5/BI
    (518-28-5/RN)
1 588-32-9/BI
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    (61736-34-3/RN)
1 618-88-2/BI
    (618-88-2/RN)
1 645-12-5/BI
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    (819805-34-0/RN)
1 819805-35-1/BI
    (819805-35-1/RN)
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1 819805-36-2/BI

(819805-36-2/RN) 1 819805-37-3/BI (819805-37-3/RN) 1 819805-38-4/BI (819805-38-4/RN) 1 819805-39-5/BI (819805-39-5/RN) 1 819805-40-8/BI (819805-40-8/RN) 1 819805-41-9/BI (819805-41-9/RN) 1 819805-42-0/BI (819805-42-0/RN) 1 819805-43-1/BI (819805-43-1/RN) 1 819805-44-2/BI (819805-44-2/RN) 1 819805-45-3/BI (819805-45-3/RN) 1 819805-46-4/BI (819805-46-4/RN) 1 819805-47-5/BI (819805-47-5/RN) 1 819805-48-6/BI (819805-48-6/RN) 1 819805-49-7/BI (819805-49-7/RN) 1 819805-50-0/BI (819805-50-0/RN) 1 819805-51-1/BI (819805-51-1/RN) 1 819805-52-2/BI (819805-52-2/RN) 1 94-74-6/BI (94-74-6/RN)1 94-75-7/BI (94-75-7/RN)1 94133-41-2/BI (94133-41-2/RN) 52 (108-30-5/BI OR 132-60-5/BI OR 151838-62-9/BI OR 15761-39-4/BI OR 171047-77-1/BI OR 176446-74-5/BI OR 1877-75-4/BI OR 1878-91-7 /BI OR 1878-94-0/BI OR 22042-71-3/BI OR 28547-08-2/BI OR 305-03-3 /BI OR 401478-57-7/BI OR 405-79-8/BI OR 47789-93-5/BI OR 4940-39-O/BI OR 499-81-0/BI OR 50996-73-1/BI OR 518-28-5/BI OR 588-32-9/B I OR 61736-34-3/BI OR 618-88-2/BI OR 645-12-5/BI OR 6470-87-7/BI OR 6559-91-7/BI OR 819805-29-3/BI OR 819805-30-6/BI OR 819805-31-7/BI OR 819805-32-8/BI OR 819805-33-9/BI OR 819805-34-0/BI OR 819805-35-1/BI OR 819805-36-2/BI OR 819805-37-3/BI OR 819805-38-4 /BI OR 819805-39-5/BI OR 819805-40-8/BI OR 819805-41-9/BI OR 819805-42-0/BI OR 819805-43-1/BI OR 819805-44-2/BI OR 819805-45-3. /BI OR 819805-46-4/BI OR 819805-47-5/BI OR 819805-48-6/BI OR 819805-49-7/BI OR 819805-50-0/BI OR 819805-51-1/BI OR 819805-52-2 /BI OR 94-74-6/BI OR 94-75-7/BI OR 94133-41-2/BI)

=> D SCAN L4

L4

L4 52 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN IN Acetic acid, 2-(4-iodophenoxy)-

· /F .

MF C8 H7 I O3

CI COM .

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L4 52 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF . C15 H19 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 52 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Acetic acid, (2,4-dichlorophenoxy)-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]1,3-dioxol-5-yl ester (9CI)

MF C30 H26 Cl2 O10

Absolute stereochemistry.

L4 52 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 52 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Acetic acid, 2-(4-fluorophenoxy)-

MF C8 H7 F O3

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L1 SSS FULL

FULL SEARCH INITIATED 09:51:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1169 TO ITERATE

100.0% PROCESSED 1169 ITERATIONS

87 ANSWERS

SEARCH TIME: 00.00.01

L5 87 SEA SSS FUL L1

=> D SCAN

L5 87 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl- β -alanyl-D-arginyl-D-arginyl-D-lysyl-D-tryptophyl-D-lysyl- (9CI)

SQL 9

MF C81 H119 N21 O20 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L5 87 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Indole-2-carboxylic acid, (5R, 5aR, 8aR, 9R)-5, 5a, 6, 8, 8a, 9-hexahydro-8-oxo-

9-(3,4,5-trimethoxyphenyl) furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)

MF C31 H27 N O9

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

MeO

L5 87 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

ОМе

R R H

IN 2-Quinolinecarboxylic acid, (5R, 5aR, 8aR, 9R)-5, 5a, 6, 8, 8a, 9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl) furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI)

OMe

MF C32 H27 N O9

Absolute stereochemistry.

PAGE 1-A



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Uploading C:\Program Files\Stnexp\Queries\10612240A.str

chain nodes :

18 24 25 26 27 28 29 30 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 19 20 21 22 23

chain bonds :

7-18 10-17 13-24 18-28, 20-26 21-25 22-27 28-29 28-30 30-31

ring bonds :

1-2 1-6 2-3 2-14 3-4 3-16 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-13

11-12 12-13 14-15 15-16 17-19 17-23 19-20 20-21 21-22 22-23

exact/norm bonds :

 $2-14 \quad 3-16 \quad 5-7 \quad 6-10 \quad 7-8 \quad 7-18 \quad 8-9 \quad 8-11 \quad 9-10 \quad 9-13 \quad 10-17 \quad 11-12 \quad 12-13 \quad 13-24$

14-15 15-16 18-28 28-29 30-31

exact bonds :

20-26 21-25 22-27 28-30

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 17-19 17-23 19-20 20-21 21-22 22-23

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS

28:CLASS 29:CLASS 30:CLASS 31:Atom

Element Count :

Node 31: Unlimited

N, N1-3

L6 STRUCTURE UPLOADED

=> D L6

L6 HAS NO ANSWERS

1.6

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> D HIS

(FILE 'HOME' ENTERED AT 09:45:20 ON 12 JUL 2007)

FILE 'REGISTRY' ENTERED AT 09:45:44 ON 12 JUL 2007

L1 STRUCTURE UPLOADED

L2 6 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:47:09 ON 12 JUL 2007.

E US2003-612240/APPS

L3 1 S E3

SEL RN L3

FILE 'REGISTRY' ENTERED AT 09:48:20 ON 12 JUL 2007

L4 52 S E1-E52

L5 87 S L1 SSS FULL

L6 STRUCTURE UPLOADED

=> S L6 SUBSET=5 FULL

5 IS NOT A VALID L#

L-numbers must be in the range L1-L999.

ENTER SUBSET L# OR (END): END

SEARCH ENDED BY USER

=> S L6 SUBSET=L5 FULL

FULL SUBSET SEARCH INITIATED 09:57:55 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 87 TO ITERATE

100.0% PROCESSED 87 ITERATIONS

80 ANSWERS

SEARCH TIME: 00.00.01

L7 80 SEA SUB=L5 SSS FUL L6

=> D SCAN L7 3

'3' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

- L7 80 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN 6-Quinolinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI)

MF C32 H27 N O9

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN

SAM - Index Name, MF, and structure - no RN FIDE - All substance data, except sequence data

IDE - FIDE, but only 50 names

SQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used

SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties

EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data

IPC -- International Patent Classification

PATS -- PI, SO

STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels

IBIB -- BIB, indented, with text labels

ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations

SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

·L7 80 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN-

IN 2-Pyridinebutanoic acid, γ-oxo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]1,3-dioxol-5-yl ester (9CI)

MF C31 H29 N O10

Absolute stereochemistry.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L7 80 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1-Piperidinyloxy, 4-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-

yl]oxy]carbonyl]-2,2,6,6-tetramethyl- (9CI)

MF C32 H38 N O10

Absolute stereochemistry. Rotation (-).

PAGE 1-A

L7 80 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1H-Indole-3-acetic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl
ester (9CI)

MF C32 H29 N O9

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> D HIS

(FILE 'HOME' ENTERED AT 09:45:20 ON 12 JUL 2007)

FILE 'REGISTRY' ENTERED AT 09:45:44 ON 12 JUL 2007 STRUCTURE UPLOADED

L1 STRUCTURE UP: L2 6 S L1 SSS SAM

•

FILE 'CAPLUS' ENTERED AT 09:47:09 ON 12 JUL 2007 E US2003-612240/APPS

L3 1 S E3 SEL RN L3

FILE 'REGISTRY' ENTERED AT 09:48:20 ON 12 JUL 2007

L4 52 S E1-E52

L5 87 S L1 SSS FULL

L6 STRUCTURE UPLOADED L7 80 S L6 FULL SUB=L5

=> S L4 AND L5

=> D SCAN 8

'8' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2-Furancarboxylic acid, 5-nitro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)

MF C27 H23 N O12

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN

SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data

IDE - FIDE, but only 50 namesSQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used ...

SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information .

BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data

IPC -- International Patent Classification

PATS -- PI, SO

STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels

IBIB -- BIB, indented, with text labels

ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations

SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 4-Quinolinecarboxylic acid, 2-phenyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)

MF C38 H31 N O9

Absolute stereochemistry.

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1(2H)-Pyrimidineacetic acid, 3,4-dihydro-6-methyl-2,4-dioxo-,
(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)

MF C29 H28 N2 O11

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,2-Pyrrolidinedicarboxylic acid, 1-(1,1-dimethylethyl)
 2-[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl] ester,
 (2S)- (9CI)
MF C32 H37 N O11

Absolute stereochemistry.

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2H-Pyrido[3,4-b]indole-2,3-dicarboxylic acid, 1,3,4,9-tetrahydro-,
2-(1,1-dimethylethyl) 3-[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]
ester (9CI)

MF C39 H40 N2 O11

Absolute stereochemistry.

PAGE 1-A

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2,3(1H)-Isoquinolinedicarboxylic acid, 3,4-dihydro-, 2-(1,1-dimethylethyl)
3-[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl] ester
(9CI)

MF . C37 H39 N O11

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 3,5-Pyridinedicarboxylic acid, bis[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl] ester (9CI)

MF C51 H45 N O18

Absolute stereochemistry.

PAGE 1-A

OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

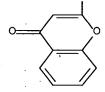
L8 8 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 4H-1-Benzopyran-2-carboxylic acid, 4-oxo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> FIL CAPLUS
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

224.00 228.14

FILE 'CAPLUS' ENTERED AT 10:04:03 ON 12 JUL 2007
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FILE 'HOME' ENTERED AT 10:41:21 ON 12 JUL 2007

=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

0.21 0.21

FILE 'REGISTRY' ENTERED AT 10:41:43 ON 12 JUL 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4 DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> ACTIVATE YANG612240/A

L1

L2 87 SEA FILE=REGISTRY SSS FUL L1

STR

=> FIL STNG

COST IN U.S. DOLLARS

SINCE FILE ENTRY

TOTAL SESSION 2.01

FULL ESTIMATED COST

1.80

FILE 'STNGUIDE' ENTERED AT 10:43:54 ON 12 JUL 2007 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 6, 2007 (20070706/UP).

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE Do you want to switch to the Registry File? Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

^{=&}gt; FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.30 2.31

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:46:42 ON 12 JUL 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4 DICTIONARY FILE UPDATES: 11 JUL 2007 HIGHEST RN 942193-36-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10612240B.str

chain nodes:
18 24 25 26 27 28 29 30 31 ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 19 20 21 22 23 chain bonds:
7-18 10-17 13-24 18-28 20-26 21-25 22-27 28-29 28-30 30-31 ring bonds:
1-2 1-6 2-3 2-14 3-4 3-16 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-13 11-12 12-13 14-15 15-16 17-19 17-23 19-20 20-21 21-22 22-23 exact/norm bonds:
2-14 3-16 5-7 6-10 7-8 7-18 8-9 8-11 9-10 9-13 10-17 11-12 12-13 13-24 14-15 15-16 18-28 28-29 30-31 exact bonds:
20-26 21-25 22-27 28-30 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 17-19 17-23 19-20 20-21 21-22 22-23

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom Element Count :
Node 31: Unlimited N,N0

L3 STRUCTURE UPLOADED

=> D L3 L3 HAS NO ANSWERS L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> S SSS L3 SUBSET=L2 SAM

SAMPLE SUBSET SEARCH INITIATED 10:47:23 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 6 TO 266
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

0 ANSWERS

L4 0 SEA SUB=L2 SSS SAM L3

=>
Uploading C:\Program Files\Stnexp\Queries\10612240C.str

chain nodes : 18 24 25 26 27 28 29 30 31 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 19 20 21 22 23 chain bonds : 7-18 10-17 13-24 18-28 20-26 21-25 22-27 28-29 28-30 30-31 ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 2-14 \quad 3-4 \quad 3-16 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 8-11 \quad 9-10 \quad 9-13$ 11-12 12-13 14-15 15-16 17-19 17-23 19-20 20-21 21-22 22-23 exact/norm bonds : . $2-14 \quad 3-16 \quad 5-7 \quad 6-10 \quad 7-8 \quad 7-18 \quad 8-9 \quad 8-11 \quad 9-10 \quad 9-13 \quad 10-17 \quad 11-12 \quad 12-13 \quad 13-24$ 14-15 15-16 18-28 28-29 30-31 exact bonds : 20-26 21-25 22-27 28-30 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 17-19 17-23 19-20 20-21 21-22 22-23

Match level :

S, S1-2

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom Element Count :
Node 31: Unlimited N,N0 0,O1-2

=> D L5 L5 HAS NO ANSWERS STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> S SSS L5 SUBSET=L2 SAM SAMPLE SUBSET SEARCH INITIATED 10:50:41 FILE 'REGISTRY' SAMPLE SUBSET SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED

6 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE** PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 6 TO 266 PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO

0 SEA SUB=L2 SSS SAM L5

0 SEA SUB=L2 SSS FUL L5

=> S SSS L5 SUBSET=L2 FULL FULL SUBSET SEARCH INITIATED 10:51:05 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED - 87 TO ITERATE

100.0% PROCESSED 87 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L7 =>

chain nodes :

18 24 25 26 27 28 29 30 31 ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 19 20 21 22 23 chain bonds:

7-18 10-17 13-24 18-28 20-26 21-25 22-27 28-29 28-30 30-31 ring bonds:

1-2 1-6 2-3 2-14 3-4 3-16 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-13 11-12 12-13 14-15 15-16 17-19 17-23 19-20 20-21 21-22 22-23 exact/norm bonds:

2-14 3-16 5-7 6-10 7-8 7-18 8-9 8-11 9-10 9-13 10-17 11-12 12-13 13-24 14-15 15-16 18-28 28-29 30-31 exact bonds:

20-26 21-25 22-27 28-30 normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6 17-19 17-23 19-20 20-21 21-22 22-23

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom Element Count :
Node 31: Unlimited 0,01-2

L8 STRUCTURE UPLOADED

=> D L8 L8 HAS NO ANSWERS L8 STR

SEARCH TIME: 00.00.01

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Structure attributes must be viewed using STN Express query preparation.

=> S SSS L8 SUBSET=L2 SAM
SAMPLE SUBSET SEARCH INITIATED 10:58:24 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 6 TO 266
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

L9 0 SEA SUB=L2 SSS SAM L8

=> S SSS L8 SUBSET=L2 FULL

FULL SUBSET SEARCH INITIATED 10:58:42 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 87 TO ITERATE

100.0% PROCESSED 87 ITERATIONS

7 ANSWERS

THE ADMINISTRATE OF THE OWNER.

SEARCH TIME: 00.00.01

L10

7 SEA SUB=L2 SSS FUL L8

=> D SCAN

L10 7 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

2-Furancarboxylic acid, (5R,5aS,8aR,9R)-5a-bromo-5,5a,6,8,8a,9-hexahydro-8oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5yl ester (9CI)

C27 H23 Br O10

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FIL CAPLU COST IN U.S. DOLLARS

SINCE FILE ENTRY SESSION

FULL ESTIMATED COST

90.75 93.06

TOTAL

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FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3 FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

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http://www.cas.org/infopolicy.html

=> S L10

L11

4 L10

=> D IBIB ABS HITSTR 1-4

L11 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:17018 CAPLUS Full-text

DOCUMENT NUMBER:

142:113818

TITLE:

Preparation of podophyllotoxin derivatives for use in

THE PROPERTY OF STREET, STREET, DESCRIPTION OF A

pharmaceutical compositions for the treatment of

cancer

INVENTOR(S):

Yang, Li-Xi

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S. Pat. Appl. Publ., 24 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.			KIND		DATE		APPL	ICAT	IÒN	NO.		D.	ATE		
US 2005	004169	A1		2005	 0106		- - US 2	- -	- 6122	- 40		2	0030	 701	
CA 2530	037	A1		2005	0217		CA 2	004-	2530	037		2	0040	630	
WO 2005014536			A2 20050217			WO 2004-US21224				20040630					
WO 2005014536			A3 20050414									20010000			
W:	AE, AG,	AL, AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR.	BW.	BY.	BZ.	CA.	CH.	
	CN, CO,	CR, CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG.	ES.	FI.	GB.	GD.	
	GE, GH,	GM, HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE.	KG.	KP.	KR.	KZ.	LC.	
•	LK, LR,	LS, LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN.	MW.	MX.	MZ.	NA.	NT.	
•	NO, NZ,	OM, PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG.	SK.	SI.	SY.	
	TJ, TM,	TN, TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC.	VN.	YU.	ZA.	ZM.	7.W	
RW:	BW, GH,	GM, KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ.	TZ.	UG.	ZM.	2W.	AM.	
	AZ, BY,	KG, KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH.	CY.	CZ.	DE.	DK.	
	EE, ES,	FI, FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL.	PT.	RO.	SE.	
	SI, SK,	TR, BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GO,	GW.	ML.	MR.	NE.	
	SN, TD,	TG						•	•	~,		,	,	,	
EP 1643	987	A2		2006	0412	1	EP 20	004-	7773	95		20	0040	630	
R:	AT, BE,														
	IE, SI,	FI, RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK	. ,	,	,	,	
PRIORITY APP							JS 20				7	A 20	030	701	
	•						WO 20						0040		

OTHER SOURCE(S): MARPAT-142:113818

Podophyllotoxin derivs., such as I [R = CO-(CH2)m-X-R1; m = 0-10; X = S, O, N, bond; R1 = substituted Ph, substituted cycloalkyl having 3 to 7 carbons forming the ring, optionally substituted fused heterocycle, naphthyl, anthraquinone, hemisuccinic acid etc.], were prepared for use as antitumor agents. When combined with suitable pharmaceutical excipients, these compds. are useful for treating various types of cancer. Thus, podophyllotoxin I (R = H) underwent an acylation reaction with F-4-C6H4OCH2CO2H using EDCI and DMAP in CH2Cl2 to give 4-(fluorophenoxyacetyl)podophyllotoxin I (R = COCH2OC6H4-4-F). The prepared podophyllotoxin derivs. were assayed in vitro for inhibition of growth of HCTl16 cells and assayed in vivo for antitumor activity in C3H/HeJ mice bearing MTG-B tumors.

IT 819805-40-8P 819805-41-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of podophyllotoxin ester derivs. for use in pharmaceutical compns. for treatment of cancer)

RN 819805-40-8 CAPLUS

CN 4H-1-Benzopyran-2-carboxylic acid, 4-oxo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

819805-41-9 CAPLUS RN

2-Furancarboxylic acid, 5-nitro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-CN 8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L11 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:372786 CAPLUS Full-text

DOCUMENT NUMBER:

138:337884

TITLE:

 3α -Bromoepipodophyllotoxin-4-substituted

derivative preparation and their anticancer activities

INVENTOR(S):

Ma, Weiyong; He, Yong; Zhang, Chunnian

PATENT ASSIGNEE(S):

Shanghai Inst. of Medical Industry, State Medicine

Management Bureau, Peop. Rep. China

SOURCE:

Faming Zhuanli Shenqing Gongkai Shuomingshu, 19 pp.

CODEN: CNXXEV

DOCUMENT TYPE:

Patent

LANGUAGE: FAMILY ACC. NUM. COUNT: Chinese

PATENT INFORMATION:

			•	
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-			
CN 1338457	Α	20020306	CN 2000-119628	20000818
PRIORITY APPLN. INFO.:			CN 2000-119628	20000818
OTHER SOURCE(S):	CASREA			

Ι

AB Title compds. I (R1 = H, alkyl, ester group, or substituted alkyl; R2 = H or methyl) were synthesized from epipodophyllotoxins via dehydration, obtained 3α , 4-anhydro-epipodophyllotoxin, dalton reaction with N-bromosuccinimide or selective hydrolysis with hydrogen bromide, giving I (R1 = H), further etherification with alc. or esterification with carboxylic acid in the presence of trifluoroborane di-Et etherate as catalyst. Title compds. have higher inhibitory effects on the growth of L1,210 and KB cells than VP-16. IT 516515-23-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

 $(3\alpha\text{-bromoepipodophyllotoxin-}4\text{-substituted derivs.}$ prepn and their bioactivities)

RN 516515-23-4 CAPLUS

2-Furancarboxylic acid, (5R,5aS,8aR,9R)-5a-bromo-5,5a,6,8,8a,9-hexahydro-8-CN oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L11 ANSWER 3 OF 4 COPYRIGHT 2007 ACS on STN CAPLUS

ACCESSION NUMBER: ·1999:534766 CAPLUS Full-text

DOCUMENT NUMBER: 132:3273

TITLE:

Synthesis and spectral characteristics of some unusual

fatty esters of podophyllotoxin

AUTHOR(S): Lie Ken Jie, M. S. F.; Mustafa, J.; Khysar Pasha, M. CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong,

Hong Kong, Peop. Rep. China

SOURCE: Chemistry and Physics of Lipids (1999), 100(1-2), 165-170

CODEN: CPLIA4; ISSN: 0009-3084 Elsevier Science Ireland Ltd.

PUBLISHER:
DOCUMENT TYPE:

Journal English

DOCUMENT TYPE:
LANGUAGE:

AB Five fatty ester derivs. of podophyllotoxin have been prepared by reacting the fatty acids with the hydroxy group of podophyllotoxin in the presence of dimethylaminopyridine and N,N-dicyclohexylcarbodiimide. The fatty acids incorporated are: 9,12-epoxy-9,11-octadecadienoic acid, octadec-11E-en-9-ynoic acid, 11,12-E-epoxy-octadec-9-ynoic acid, octadeca-9Z,11E-dienoic acid and 9,10-dibromooctadecanoic acid. Average yields were >95% and the structures of the products were confirmed by a combination of NMR spectroscopic and mass spectrometric analyses.

IT 251109-11-2P 251109-13-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and spectral characteristics of some fatty esters of podophyllotoxin)

RN 251109-11-2 CAPLUS

CN 2-Furanoctanoic acid, 5-hexyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251109-13-4 CAPLUS

ON 9-Decynoic acid, 10-(3-hexyloxiranyl)-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Me (CH₂) 5
$$C = C$$
 (CH₂) 7 O

REFERENCE COUNT:

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1998:291310 CAPLUS Full-text

DOCUMENT NUMBER:

129:175488

TITLE:

Synthesis of epipodophyllotoxin carboxylates and

antitumor activity in vitro

AUTHOR(S):

CORPORATE SOURCE:

Pan, Jianlin; Wang, Yanguang; Chen, Yaozhu Department of Chemistry, Zhejiang University,

Hangzhou, 310027, Peop. Rep. China

SOURCE:

Yaoxue Xuebao (1997), 32(12), 898-901

CODEN: YHHPAL; ISSN: 0513-4870

PUBLISHER:

Chinese Academy of Medical Sciences, Institute of

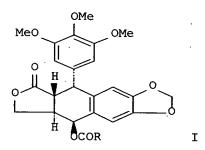
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DOCUMENT TYPE:

LANGUAGE:

Journal

GΙ



AB Epipodophyllotoxin carboxylates [I; R = Ph, o-acetoxyphenyl, m-tolyl, styryl, 3,5-dinitrophenyl, 2-furyl, 2-furylethenyl] were prepared via reacting podophyllotoxin with the appropriate organic acids under the catalysis of BF3.Et2O. The compds. showed significant antitumor activities against mouse leukemia P388 and human stomach cancer SGC-7901 in pharmacol. tests in vitro. IT 211615-64-4P 211615-65-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of antitumor epipodophyllotoxin carboxylates)

RN 211615-64-4 CAPLUS

CN 2-Furancarboxylic acid, (5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 211615-65-5 CAPLUS

CN 2-Propenoic acid, 3-(2-furanyl)-, (5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

=> SAVE L10 YAN612440/A TEMP
ANSWER SET NOT SAVED.
THE ANSWER SET WAS CREATED IN FILE 'REGISTRY'.
USE THE FILE COMMAND TO CHANGE TO THE CORRECT FILE.
Answer sets must be saved in the same file in which they were created.

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(FILE 'HOME' ENTERED AT 10:41:21 ON 12 JUL 2007)

FILE 'REGISTRY' ENTERED AT 10:41:43 ON 12 JUL 2007

ACTIVATE YANG612240/A

STN INTERNATIONAL LOGOFF AT 11:01:30 ON 12 JUL 2007

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L2 87 SEA FILE=REGISTRY SSS FUL L1		
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(FILE 'HOME' ENTERED AT 09:45:20 ON 12 JUL 2007)

FILE 'REGISTRY' ENTERED AT 09:45:44 ON 12 JUL 2007

L1 STRUCTURE UPLOADED

L2 6 S L1 SSS SAM

FILE 'CAPLUS' ENTERED AT 09:47:09 ON 12 JUL 2007

E US2003-612240/APPS

L3 1 S E3 SEL RN L3

FILE 'REGISTRY' ENTERED AT 09:48:20 ON 12 JUL 2007

L4 52 S E1-E52

L5 87 S L1 SSS FULL

L6 STRUCTURE UPLOADED

L7 80 S L6 FULL SUB=L5

L8 8 S L4 AND L5

FILE 'CAPLUS' ENTERED AT 10:04:03 ON 12 JUL 2007

=> S L7

L9 19 L7

=> FIL STNG

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.47 228.61

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 6, 2007 (20070706/UP).

=> FIL CAPLUS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.60 229.21

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FILE COVERS 1907 - 12 Jul 2007 VOL 147 ISS 3 FILE LAST UPDATED: 11 Jul 2007 (20070711/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

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=> D IBIB ABS HITSTR L9 1-19

L9 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2006:263203 CAPLUS Full-text

DOCUMENT NUMBER: 144:460304

TITLE: Synthesis and biological evaluation of new

spin-labeled derivatives of podophyllotoxin

AUTHOR(S): Jin, Yan; Chen, Shi-Wu; Tian, Xuan

CORPORATE SOURCE: State Key Laboratory of Applied Organic Chemistry,

Lanzhou University, Lanzhou, 730000, Peop. Rep. China

SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(9),

3062-3068

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:460304

In order to find compds. with superior bioactivity and less toxicity, a series of spin-labeled podophyllotoxin derivs. were synthesized and tested for the partition coeffs. and cytotoxicity against P-388 and A-549. Furthermore, we also determined antioxidant activities of target mol. in tissues of SD rats by the TBA method. Results revealed that most synthesized compds. showed more significant cytotoxicity against P-388 and A-549 in vitro than VP-16. Among them, the tetramethylpiperidine derivative exhibited most potent cytotoxicity against P-388 and A-549 cells (IC50 is <0.01 and 0.13 µM, resp.). Also, the antioxidative activities showed that the modified compds. of 4'-demailylepipodophyllotoxin are higher than those of podophyllotoxin series. The relationship between the cytotoxicity and antioxidative activity discussed.

IT 193404-42-1P 886757-90-0P 886757-91-1P 886757-92-2P 886757-93-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(synthesis and biol. evaluation of spin-labeled derivs. of podophyllotoxin)

RN 193404-42-1 CAPLUS

CN 1H-Pyrrol-1-yloxy, 3-[[[(5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-

yl]oxy]carbonyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)
Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

ме Ме

OMe

R R H

Me

RN 886757-90-0 CAPLUS

CN 1H-Pyrrol-1-yloxy, 3-[[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

OMe

Absolute stereochemistry. Rotation (-).

PAGE 1-A

Me Me

RN 886757-91-1 CAPLUS

CN 1(2H)-Pyridinyloxy, 4-[[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-3,6-dihydro-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

L Me

RN 886757-92-2 CAPLUS

CN 1-Pyrrolidinyloxy, 3-[[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

PAGE 2-A

Mé

RN 886757-93-3 CAPLUS

CN 1-Piperidinyloxy, 4-[[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

OMe

IT 886758-00-5P 886758-01-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis and biol. evaluation of spin-labeled derivs. of podophyllotoxin)
RN 886758-00-5 CAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 2,5-dihydro-1-hydroxy-2,2,5,5-tetramethyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

Me Me

RN 886758-01-6 CAPLUS
CN 1H-Pyrrole-3-carboxylic acid, 2,5-dihydro-1-hydroxy-2,2,5,5-tetramethyl-,
(5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)
(CA INDEX NAME)

PAGE 2-A

Me Me

REFERENCE COUNT:

52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:133229 CAPLUS Full-text

DOCUMENT NUMBER:

145:7931

TITLE:

Method of preparation pyridyl podophyllotoxin

compounds for preparation insecticide

INVENTOR(S):

Gao, Rong; Xiao, Hang; Di, Xudong; Liu, Yanqing

PATENT ASSIGNEE(S):

Nanjing Medical University, Peop. Rep. China

SOURCE:

Faming Zhuanli Shenqing Gongkai Shuomingshu, 25 pp.

CODEN: CNXXEV

DOCUMENT TYPE:

Patent

LANGUAGE:

Chinese

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		·		
CN 1663955	. A	20050907	CN 2005-10037723	20050202
PRIORITY APPLN. INFO.:			CN 2005-10037723	20050202
OTHER SOURCE(S):	CASRE	ACT 145:7931;	MARPAT 145:7931	
GT				

AB The structures of pyridyl podophyllotoxin compds. I and II [R = pyridyl group] are presented. The method comprises stirring organic acid and 4'-demethyl podophyllotoxin (at mole ratio of 1:1) in the presence of catalyst (4-dimethylaminopyridine) in anhydrous organic solvent (ether, dichloromethane, carbon tetrachloride, chloroform) at room temperature for 5-10 mins; then adding DCC and reacting for 1-3 h; filtering, concentrating filtrate; purifying on column and recrystg. to give product. The organic acid can be isonicotinic acid, nicotinic acid, picolinic acid, 2-chloro-nicotinic acid, 6-chloro-nicotinic acid, 5-bromo-nicotinic acid. The pyridyl podophyllotoxin compds. can be used for preparation insecticide.

IT 608524-44-3P 608524-47-6P 888029-85-4P 888029-86-5P 888029-87-6P 888029-88-7P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridylpodophyllotoxin derivs. as insecticide) 608524-44-3 CAPLUS

RN 608524-44-3 CAPLUS
CN 2-Pyridinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 608524-47-6 CAPLUS

CN 3-Pyridinecarboxylic acid, 6-chloro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-

1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

l OMe

RN 888029-85-4 CAPLUS

CN 4-Pyridinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 888029-86-5 CAPLUS

CN 3-Pyridinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 888029-87-6 CAPLUS

CN 3-Pyridinecarboxylic acid, 2-chloro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 888029-88-7 CAPLUS

CN 3-Pyridinecarboxylic acid, 5-bromo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L9 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:54534 CAPLUS Full-text

DOCUMENT NUMBER:

144:170828

TITLE:

Preparation of epipodophyllotoxin derivatives and

their use as insecticides

INVENTOR(S):

Li, Guangze; Feng, Juntao; Hao, Shuanghong; He, Jun;

Duan, Ling; Zhang, Xing

PATENT ASSIGNEE(S):

Biorational Pesticide Research and Service Center,

Northwest Sci-Tech University of Agriculture and

Forestry, Peop. Rep. China

SOURCE:

Faming Zhuanli Shenqing Gongkai Shuomingshu, 67 pp.

CODEN: CNXXEV

DOCUMENT TYPE:

Patent

LANGUAGE:

Chinese

FAMILY ACC. NUM. COUNT:

: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1590388	Α	20050309	CN 2003-10105870	20031030
PRIORITY APPLN. INFO.:			CN 2003-10105870	20031030
GI				

AB Epipodophyllotoxin derivs. I [wherein R = acetyl, propionyl, mercapto, etc.] were prepared and found to have insecticidal activity toward Mythimna separata Walker, Plutella xylostella and Pieris rapae. Therefore, I are useful for the treatment or prevention of these insects.

IT 874661-48-0P 874661-49-1P
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
 SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of epipodophyllotoxin derivs. and their use as insecticides) 874661-48-0 CAPLUS

RN 874661-48-0 CAPLUS
CN 3-Pyridinecarboxylic acid, (5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 874661-49-1 CAPLUS

CN 4-Pyridinecarboxylic acid, (5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:17018 CAPLUS Full-text

DOCUMENT NUMBER: 142:113818

TITLE: Preparation of podophyllotoxin derivatives for use in

pharmaceutical compositions for the treatment of

cancer

INVENTOR(S):
Yang, Li-Xi

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 24 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	rent :				KIN		DATE			APPL 						ATE	
	2005						2005									0030	
CA	2530	037			A1		2005	0217		CA 2	004-	2530	037		2	0040	630
WO	2005	0145	36		A2		2005	0217		WO 2	004-	US21	22.4		2	0040	630
WO	2005	0145	36		А3		2005	0414									
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	.FI,	GB,	GD,
		GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
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							GR,										
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		SN,	TD,	TG													
EP	1643	987			A2		2006	0412		EP 2	004-	7773	95		2	0040	630
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		IE,	SI,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK				
PRIORIT	Y APP	LN.	INFO	.:						US 2	003-	6122	40		A 2	0030	701
									,	WO 2	004-	US21:	224	I	W 2	0040	630
OTHER SO	OURCE	(S):			MAR	PAT	142:	1138	18								•

AB Podophyllotoxin derivs., such as I [R = CO-(CH2)m-X-R1; m = 0-10; X = S, O, N, bond; R1 = substituted Ph, substituted cycloalkyl having 3 to 7 carbons forming the ring, optionally substituted fused heterocycle, naphthyl,

anthraquinone, hemisuccinic acid etc.], were prepared for use as antitumor agents. When combined with suitable pharmaceutical excipients, these compds. are useful for treating various types of cancer. Thus, podophyllotoxin I (R = H) underwent an acylation reaction with F-4-C6H4OCH2CO2H using EDCI and DMAP in CH2Cl2 to give 4-(fluorophenoxyacetyl)podophyllotoxin I (R = COCH2OC6H4-4-F). The prepared podophyllotoxin derivs. were assayed in vitro for inhibition of growth of HCTl16 cells and assayed in vivo for antitumor activity in C3H/HeJ mice bearing MTG-B tumors.

IT 819805-43-1P 819805-44-2P 819805-46-4P
819805-49-7P 819805-50-0P 819805-52-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of podophyllotoxin ester derivs. for use in pharmaceutical compns. for treatment of cancer)

RN 819805-43-1 CAPLUS

CN 4-Quinolinecarboxylic acid, 2-phenyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 819805-44-2 CAPLUS
CN 1(2H)-Pyrimidineacetic acid, 3,4-dihydro-6-methyl-2,4-dioxo-,
(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)
(CA INDEX NAME)

RN 819805-46-4 CAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 1-(1,1-dimethylethyl)
2-[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl] ester,
(2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

RN 819805-50-0 CAPLUS

CN 2,3(1H)-Isoquinolinedicarboxylic acid, 3,4-dihydro-, 2-(1,1-dimethylethyl) 3-[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl] ester (9CI) (CA INDEX NAME)

PAGE 2-A

819805-52-2 CAPLUS

RN

CN 3,5-Pyridinedicarboxylic acid, bis[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl] ester (9CI) (CA INDEX NAME)

L9 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:779090 CAPLUS Full-text

DOCUMENT NUMBER:

139:292103

TITLE:

Preparation of new podophyllotoxin derivatives and

their therapeutic application

INVENTOR(S):

Potier, Pierre; Kerkar, Brahim

PATENT ASSIGNEE(S):

Fr.

1

SOURCE:

Fr. Demande, 40 pp.

CODEN: FRXXBL

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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FR 2837824	A1	20031003	FR 2002-3903	20020328
FR 2837824	В1	20060303	•	
WO 2003082875	A2 .	20031009	WO 2003-FR983	20030328

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WO 2003082875
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                                20031013
                                            AU 2003-244727
     AU 2003244727
                                                                    20030328
PRIORITY APPLN. INFO.:
                                            FR 2002-3903
                                                                 A 20020328
                                            WO 2003-FR983
                                                                 W .20030328
                         CASREACT 139:292103; MARPAT 139:292103
OTHER SOURCE(S):
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GI

AΒ The invention relates to podophyllotoxin derivs. I [R = CH2NHC(:O)R2,CH(OH)CHR17NHC(:O)R3, CH(OH)CHPhNHC(:O)R3, pyrrolyl-, pyridyl-, imidazolyl-,

pyrazinylalkylene or -vinyl, N-oxopyridyl, quinolinyl, oxodihydroquinolinyl, etc.; R2 = (un)substituted pyrrole, imidazole, pyridine, pyrazine, indole, Ph, naphthalene, quinoline or thiazole groups; R3 = O-(C1-4-alkyl),

(un) substituted Ph (substituted with halogen or OMe); R17 = pyridyl, C1-4alkyl, (un) substituted Ph (substituted with halogen, NO2, OH or OMe)], their bases or addition salts with pharmaceutically acceptable acids, in the form of enantiomers, diastereoisomers, or their mixts. (including racemic mixts.).

The method of preparation and its therapeutic application, particularly against cancer, is described. Thus, I (R = 2-pyridyl) was prepared from podophyllotoxin via reaction with pyridine-2-carboxylic acid in CH2Cl2

containing DMAP and 1-[3- (dimethylamino)propyl]-3-ethylcarbodiimide hydrochloride. The cytotoxicity of I (@ 10-100 nM) vs. human tumor cell lines

(A549, HT-29, KB, KB-VMH, KB-VP2, MDA-MB-231, SK-N-SH) was tested (no data). 608524-41-0P 608524-44-3P 608524-45-4P

ΙT 608524-46-5P 608524-47-6P 608524-48-7P

608524-49-8P 608524-50-1P 608524-51-2P

608524-52-3P 608524-53-4P 608524-54-5P

608524-55-6P 608524-56-7P 608524-57-8P

608524-58-9P 608524-59-0P 608524-60-3P

608524-61-4P 608524-62-5P 608524-63-6P

608524-64-7P 608524-65-8P 608524-66-9P 608524-67-0P 608524-68-1P 608524-69-2P

Absolute stereochemistry.

RN 608524-44-3 CAPLUS

CN 2-Pyridinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 608524-45-4 CAPLUS

CN 3-Pyridinecarboxylic acid, 6-methyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-

hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

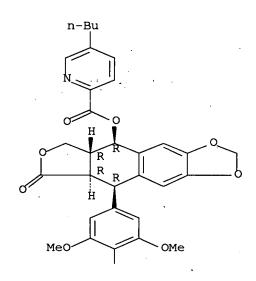
PAGE 2-A

OMe

RN 608524-46-5 CAPLUS

CN 2-Pyridinecarboxylic acid, 5-butyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

PAGE 1-A



OMe.

RN 608524-47-6 CAPLUS

CN 3-Pyridinecarboxylic acid, 6-chloro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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PAGE 2-A

OMe

RN 608524-48-7 CAPLUS

CN 2-Pyridinecarboxylic acid, 3-hydroxy-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

RN 608524-49-8 CAPLUS
CN 3-Pyridinecarboxylic acid, 1,2-dihydro-2-oxo-, (5R,5aR,8aR,9R)5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap
htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-50-1 CAPLUS
CN 2-Pyridinecarboxylic acid, 3-(phenylmethoxy)-, (5R,5aR,8aR,9R)5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap
htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

RN 608524-51-2 CAPLUS

CN 2-Pyridineacetic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-52-3 CAPLUS

CN 3-Pyridineacetic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

RN 608524-53-4 CAPLUS

CN 4-Pyridineacetic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-54-5 CAPLUS

CN 3-Pyridinepropanoic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

RN 608524-55-6 CAPLUS

CN Pyrazinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-56-7 CAPLUS

CN 2-Propenoic acid, 3-(3-pyridinyl)-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 608524-57-8 CAPLUS

CN 2-Propenoic acid, 3-(4-pyridinyl)-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

RN 608524-58-9 CAPLUS

CN 2-Propenoic acid, 3-(1-methyl-1H-imidazol-4-yl)-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 608524-59-0 CAPLUS

CN 3-Pyridinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, 1-oxide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-60-3 CAPLUS

CN 1H-Indole-2-carboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

RN 608524-61-4 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-nitro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-62-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-nitro-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

RN 608524-63-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-hydroxy-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-64-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-(phenylmethoxy)-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-65-8 CAPLUS

CN 1H-Indole-3-acetic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

RN 608524-66-9 CAPLUS

CN 1H-Indole-3-propanoic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-67-0 CAPLUS

CN 1H-Indole-3-butanoic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

RN 608524-68-1 CAPLUS

CN 1H-Indole-3-acetic acid, 5-bromo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-69-2 CAPLUS

CN 1H-Indole-3-acetic acid, 1-methyl-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Мe

RN 608524-70-5 CAPLUS

CN lH-Indole-3-acetic acid, α -[[(1,1-dimethylethoxy)carbonyl]amino]-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, (α R)- (9CI) (CA INDEX NAME)

RN 608524-71-6 CAPLUS

CN 1H-Indole-3-acetic acid, 5-methoxy-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608524-89-6 CAPLUS

CN 6-Quinolinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

OMe

H

MeO

RN 608524-90-9 CAPLUS

CN 2-Quinolinecarboxylic acid, 4-hydroxy-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

RN 608524-91-0 CAPLUS

CN 4-Quinolinecarboxylic acid, 1,2-dihydro-2-oxo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

RN 608524-93-2 CAPLUS
CN 4-Quinolinecarboxylic acid, 1,2,3,4-tetrahydro-2-oxo-,
(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

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RN 608524-96-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-,
(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-
trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)
(CA INDEX NAME)
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RN 608524-98-7 CAPLUS

CN 4-Thiazoleacetic acid, 2-[(pyrazinylcarbonyl)amino]-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 608525-01-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-[(2-pyridinylcarbonyl)amino]-,
(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI)
(CA INDEX NAME)

RN 608525-03-7 CAPLUS

CN 4-Thiazoleacetic acid, 2-[(1H-indol-3-ylacetyl)amino]-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

CN 2-Quinolinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 609356-69-6 CAPLUS

CN 3-Quinolinecarboxylic acid, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-ylester (9CI) (CA INDEX NAME)

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2000:351544 CAPLUS Full-text

DOCUMENT NUMBER:

TITLE:

Modified and truncated penetratin derivatives as membrane translocation carriers for drug transport

Fischer, M. Peter; Zhelev, Nikolai

INVENTOR(S):

Cyclacel Limited, UK

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	CENT 1	NO.			KIN	D	DATE			APPL	ICAT:	ION I	NO.		D	ATE	
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WO	2000	0294	27		A2		2000	0525	1	WO 1	999-	GB37	50		. 1	9991	111
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		IN,	IS,	JP,	ΚĖ,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,
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		SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VN,	YU,	ZA,	ZW	
	RW:	GH.	GM.	KE.	LS.	MW.	SD.	SL.	SZ.	TZ.	UG.	ZW.	AT.	BE.	CH.	CY.	DE.

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             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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PRIORITY APPLN. INFO.:
                                             GB 1998-25000
                                                                 A 19981113
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                                                                 A 19981113
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                                                                    19990204
                                             GB 1999-2525
                                                                 Α
                                             GB 1999-14578
                                                                 A 19990622
                                             WO 1999-GB3750
                                             US 1999-438460
                                                                 A3 19991112
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The invention relates to modified and truncated forms of the membrane transport vector penetratin, a peptide comprising residues 45-58 of the Antennapedia homeodomain protein. Such truncated forms include 7-mer peptides that may in themselves include further variation. Such smaller or truncated forms of penetratin are advantageous in that they are more acceptable to the pharmaceutical industry as delivery carrier moieties, by virtue of the carrier-cargo conjugate having an advantageous immunogenicity, solubility, and clearance, and in some cases advantageous efficacy as compared to using a conjugate comprised of full length penetratin. Carrier moieties are synthetically linked to a cargo moiety selected from p21WAF-derived peptides, p16-derived peptides or the drugs roscovitine, taxol, or a podophyllotoxin. The truncated penetratin-podophyllotoxin conjugate, for example, is more effective in terms of anti-proliferative activity on tumor cells while exhibiting lower generalized toxicity.

IT 254893-96-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(modified and truncated penetratin derivs. as membrane translocation carriers for drug transport)

RN 254893-96-4 CAPLUS

CN 1H-Pyrrole-1-propanoic acid, 2,5-dihydro-2,5-dioxo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

IT 254894-03-6P 254894-06-9P 254894-57-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(modified and truncated penetratin derivs. as membrane translocation carriers for drug transport)

RN 254894-03-6 CAPLUS

CN L-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-β-alanyl-L-arginyl-L-arginyl-L-tryptophyl-L-lysyl- (9CI) (CA INDEX NAME)

RN 254894-06-9 CAPLUS

CN D-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-β-alanyl-D-arginyl-D-arginyl-D-tryptophyl-D-lysyl-(9CI) (CA INDEX NAME)

PAGE 1-A

RN254894-57-0 CAPLUS

L-Cysteinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-hexahydrCN (3,4,5-trimethoxyphenyl) furo [3',4':6,7] naphtho [2,3-d]-1,3-dioxol-5-yl] oxy]-13-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-L-arginyl-L-arginyl-Lmethionyl-L-lysyl-L-tryptophyl-L-lysyl-S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-(9CI) (CA INDEX NAME)

OMe MeO. OMe

PAGE 1-C

L9 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2000:34769 CAPLUS Full-text

DOCUMENT NUMBER:

132:93654

TITLE:

Preparation of peptide derivatives for improved

delivery of drug therapeutic agents

INVENTOR(S):

Fischer, Peter Martin; Wang, Shudong

PATENT ASSIGNEE(S):

SOURCE:

Cyclacel Limited, UK PCT Int. Appl., 115 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.				DATE					
WO 2000001417				A1 20000113			WO 1999-GB1957					10000633					
WO 2000001417			ΑI	A1 20000113			WO 1999-GD195/				19990622						
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		DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,
		JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,
		MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,
		TM,	TR,	TT,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW					

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
             ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
             CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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                                 20000906
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                           A1
                                 20010425
                                              EP 1999-928071
                                                                      19990622
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                           B1
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             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     JP 2002519392
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                                 20020702
                                              JP 2000-557863
                                                                      19990622
     HU 200300246
                           A2
                                 20030528
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                                 20050928
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                                 20041015
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                                 20060131
PRIORITY APPLN. INFO.:
                                              GB 1998-14527
                                                                      19980703
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                                                                      19990622
                                                                   W
                                              US 1999-346847
                                                                   A1 19990702
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AB The present invention relates to a novel drug delivery system for use in the improved delivery of drug therapeutic agents into target cells. The system comprises a drug moiety linked to a carrier moiety wherein the carrier moiety comprises a homeobox peptide or its fragment or derivative Thus, {[4-[N-(2,4-diamino-6-pteridinylmethyl)-N-methylamino]benzoyl]-Glu- Gly- β -Ala}4-Lys2-Lys- β -Ala-Arg-Gln-Ile-Lys-Ile-Trp-Phe-Gln-Asn- Arg-Arg-Met-Lys-Trp-Lys-Lys-OH was prepared by the solid-phase method and assayed for in vitro cytotoxicity.

IT 254893-96-4P 254893-97-5P 254893-99-7P

254894-00-3P 254894-02-5P 254894-03-6P

254894-06-9P 254894-57-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of peptide derivs. for improved delivery of drug therapeutic agents)

RN 254893-96-4 CAPLUS

CN 1H-Pyrrole-1-propanoic acid, 2,5-dihydro-2,5-dioxo-, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

RN 254893-97-5 CAPLUS

CN L-Lysine, S-[1-[3-[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-L-arginyl-L-glutaminyl-L-isoleucyl-L-lysyl-L-isoleucyl-L-tryptophyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-arginyl-L-arginyl-L-methionyl-L-lysyl-L-tryptophyl-L-lysyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

$$H_2N$$
 (CH₂) 4 S H_2N (CH₂) 4 R

PAGE 2-C

OMe

RN 254893-99-7 CAPLUS
CN Glycinamide, N-[6-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]-1-oxohexyl]-β-alanyl-L-arginyl-L-glutaminyl-L-isoleucyl-L-lysyl-L-isoleucyl-L-tryptophyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-arginyl-L arginyl-L-methionyl-L-lysyl-L-tryptophyl-L-lysyl-L-lysylglycyl-S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-

Absolute stereochemistry.

(9CI) (CA INDEX NAME)

HN=

PAGE 1-B

PAGE 1-C

PAGE 1-E

PAGE 2-E

RN 254894-00-3 CAPLUS

CN L-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-L-arginyl-L-glutaminyl-L-isoleucyl-L-lysyl-L-isoleucyl-L-tryptophyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-arginyl-L-arginyl-L-methionyl-L-lysyl-L-tryptophyl-L-lysyl-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 1-C

RN 254894-02-5 CAPLUS

CN D-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-D-arginyl-D-glutaminyl-D-isoleucyl-D-lysyl-D-isoleucyl-D-tryptophyl-D-phenylalanyl-D-glutaminyl-D-asparaginyl-D-arginyl-D-arginyl-D-norleucyl-D-lysyl-D-tryptophyl-D-lysyl-(9CI) (CA INDEX NAME)

PAGE 1-C

PAGE 1-D

RN 254894-03-6 CAPLUS

CN L-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-β-alanyl-L-arginyl-L-arginyl-L-methionyl-L-lysyl-L-tryptophyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 254894-06-9 CAPLUS

CN D-Lysinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-

 $3-oxopropyl]-2, 5-dioxo-3-pyrrolidinyl]-L-cysteinyl-<math>\beta$ -alanyl-D-arginyl-D-arginyl-D-tryptophyl-D-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 254894-57-0 CAPLUS

CN L-Cysteinamide, S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-L-cysteinyl-L-arginyl-L-arginyl-L-methionyl-L-lysyl-L-tryptophyl-L-lysyl-L-lysyl-S-[1-[3-[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]-3-oxopropyl]-2,5-dioxo-3-pyrrolidinyl]-(9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 1-C

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:568594 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 132:15517

TITLE: Drug delivery of anticancer agents: water soluble

4-polyethylene glycol derivatives of the lignan,

podophyllotoxin

AUTHOR(S): Greenwald, R. B.; Conover, C. D.; Pendri, A.; Choe, Y.

H.; Martinez, A.; Wu, D.; Guan, S.; Yao, Z.; Shum, K.

L.

CORPORATE SOURCE: Research and Development, Department of Organic and

Medicinal Chemistry, Enzon, Inc., Piscataway, NJ, USA

Journal of Controlled Release (1999), 61(3), 281-294

CODEN: JCREEC; ISSN: 0168-3659

PUBLISHER: Elsevier Science Ireland Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

This paper reports on the synthesis and in vivo oncolytic activity of a series of water-soluble acyl derivs. of polyethylene glycol (PEG) conjugated podophyllotoxin. Some analogs of the polymer conjugate showed significantly better activity in a murine leukemia model than native podophyllotoxin suspended in an intralipid emulsion. Addnl., when tested i.v. against a solid lung tumor (A549) model, some conjugated analogs were equivalent to the podophyllotoxin/intralipid emulsion, while those compds. demonstrating slower rates of plasma hydrolysis (in vitro) appeared to cause greater toxicity. There appeared to be an overall correlation between the in vivo antitumor activity of the conjugate and its rate of hydrolysis in vitro, with those showing faster release possessing greater antitumor activity. In conclusion, the solubilization and predictable release of podophyllotoxin from a PEG carrier was achieved and resulted in some derivs. demonstrating, at a min., equivalency with podophyllotoxin when administered on an equal molar basis. Further studies may be warranted to assess the PEG-conjugates pharmacokinetics and therapeutic indexes in leukemic models.

IT 251565-08-9P

SOURCE:

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antitumor activity of water soluble PEG derivs. of podophyllotoxin)

RN 251565-08-9 CAPLUS

CN Poly(oxy-1,2-ethanediyl), $\alpha-[2-[(2S)-2-[[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)]]] furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-1-pyrrolidinyl]-2-oxoethyl]- <math>\omega-[2-[(2S)-2-[[[(5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)]]]]$ furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-1-pyrrolidinyl]-2-oxoethoxy]- (9CI) (CA INDEX NAME)

MeO OMe MeO MeO MeO NeO CH2-
$$CH_2$$
- CH_2 -

PAGE 1-B

IT 251565-03-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antitumor activity of water soluble PEG derivs. of podophyllotoxin) $\,$

RN 251565-03-4 CAPLUS

CN L-Proline, (5R,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1997:457449 CAPLUS Full-text

DOCUMENT NUMBER:

127:149030

TITLE:

Syntheses and structure-activity relationship of podophyllotoxin derivatives as potential anticancer

drugs

AUTHOR(S):

Wang, Yan-Guang; Tao, Lan; Pan, Jian-Lin; Shi,

Jian-Feng; Chen, Yao-Zu

CORPORATE SOURCE:

Dep. Chem., Zhejiang University, Hangzhou, 310027,

Peop. Rep. China

SOURCE:

Gaodeng Xuexiao Huaxue Xuebao (1997), 18(7), 1061-1066

CODEN: KTHPDM; ISSN: 0251-0790

PUBLISHER:

Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE:

Journal

LANGUAGE:

Chinese

GΙ

AB Thirteen 4 β -substituted podophyllotoxin derivs. I (R1 = H, Me; R2 = R3NH, R3O, R4CONH, 3,5-(NO2)2C6H3CONH, R4CO2, etc.) were prepared from podophyllotoxin or 4'-demethylpodophyllotoxin and evaluated for antitumor activity against mouse leukemia P388 in vivo and human stomach carcinoma SGC-7901 in ivtro. Structure activity relationship was discussed. These results demonstrate the importance of 4'-phenolic hydroxyl group, and suggest further elaboration of 4 β -nitrogen-containing substitution to simplify and optimize the structure of this class of anticancer compds.

IT 193404-42-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(syntheses and structure-activity relationship of anticancer podophyllotoxin derivs.)

RN 193404-42-1 CAPLUS

CN 1H-Pyrrol-1-yloxy, 3-[[[(5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-2,5-dihydro-2,2,5,5-tetramethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

Me Me

L9 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1997:422746 CAPLUS Full-text

DOCUMENT NUMBER:

127:144745

TITLE:

New spin labeled analogs of podophyllotoxin as

potential antitumor agents

AUTHOR(S):

Wang, Yan-guang; Pan, Jian-lin; Shi, Jian-feng; Chen,

Yao-zu

CORPORATE SOURCE:

Department Chemistry, Zhejiang University, Hangzhou,

310027, Peop. Rep. China

SOURCE: Life Sciences (1997), 61(5), 537-542

CODEN: LIFSAK; ISSN: 0024-3205

PUBLISHER:
DOCUMENT TYPE:

Elsevier Journal

DOCUMENT T

English

Four new nitroxyl labeled derivs. of podophyllotoxin, 4-(2,2,6,6- tetramethyl-1-oxyl-4-piperidyl)oxy-epipodophyllotoxin, 4-(2,2,6,6-tetramethyl-1-oxyl-4-piperidyl)oxy-4'- demethylepipodophyllotoxin, 4-(2,2,5,5-tetramethyl-1-oxyl-3-pyrrolinyl)formyloxy-epipodophyllotoxin and 4-(2,2,5,5-tetramethyl-1-oxyl-3-pyrrolinyl)formyloxy-4'-demethylepipodophyllotoxin, have been synthesized and evaluated for their antitumor activity in vitro. The 4'-demethyl-epipodophyllotoxins showed superior activity to the clin. used etoposide (VP-16) in their inhibition of leukemia P388, lung cancer A549 and stomach carcinoma SGC-7901 cells. The 4'-demethyl-epipodophyllotoxins was more active than the eipodophyllotoxins lacking a free phenolic hydroxyl group at C-4'.

IT 193404-42-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of new spin labeled analogs of podophyllotoxin as potential antitumor agents)

RN 193404-42-1 CAPLUS

CN 1H-Pyrrol-1-yloxy, 3-[[[(5S,5aR,8aR,9R)-5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl]oxy]carbonyl]-2,5-dihydro-2,2,5,5-tetramethyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

L9 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:524013 CAPLUS Full-text

DOCUMENT NUMBER: 117:124013

TITLE: Different mechanisms of action of long chain fatty

acid esters of podophyllotoxin and esters of

epipodophyllotoxin against P388 lymphocytic leukemia

in mice

AUTHOR(S): Nagao, Yoshimitsu; Mustafa, Jamal; Sano, Shiqeki;

Ochiai, Masahito; Tashiro, Tazuko; Tsukagoshi, Shigeru

CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokushima, Tokushima, 770,

Japan

SOURCE: Medicinal Chemistry Research (1991), 1(4), 295-9

CODEN: MCREEB; ISSN: 1054-2523

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Among podophyllotoxin and epipodophyllotoxin esters of long chain unsatd. or polyhydroxy fatty acids, esters of the former exhibited significant or strong activity against P388 lymphocytic leukemia inoculated into mice. Structure-activity relations are discussed.

IT 143361-59-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(neoplasm-inhibiting activity of, structure in relation to)

RN 143361-59-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[(1-oxo-9,12-octadecadienyl)oxy]ethyl]-, 5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester, [5R-[5 α (9Z,12Z),5a α ,8a.beta .,9 α]]- (9CI) (CA INDEX NAME)

PAGE 1-A

ANSWER 12 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

150

ACCESSION NUMBER:

1990:7272 CAPLUS Full-text

DOCUMENT NUMBER:

112:7272

TITLE:

L9

Preparation and testing of podophyllotoxin derivatives

as neoplasm inhibitors

INVENTOR(S):

Nagao, Yoshuki; Tsukagoshi, Shigeru; Nakamura,

Tadatake

PATENT ASSIGNEE(S):

Daiichi Seiyaku Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01117885	Α	19890510	JP 1987-275213	19871030
PRIORITY APPLN. INFO) .:		JP 1987-275213	19871030
OTHER SOURCE(S):	MARPAT	112:7272		•
GI				

$$\begin{array}{c|c}
0 & Y \\
X & R^{2}
\end{array}$$

Title compds. I [R1,R2,R3 = alkoxy; X = halo, H; Y = halo, OH, OCOR4; R4 = (hydroxyalkyl-, cyclic amino-, or benzodioxolyl-substituted) cyclic amino, (cyclic amino-substituted) alkyl amino, (≥1 OH-substituted) (un)saturated hydrocarbyl; except a combination of X = H and Y = OH] are prepared Podophyllotoxin II (Y = OH) was treated with ClCO2Ph in CH2Cl2 in the presence of pyridine to give II (Y = OCO2Ph), which was treated with 2-piperazinoethanol in CH2Cl2 to give II [Y = 4-(2- hydroxyethyl)piperazino]. II [Y = OCO(CH2)7CH:CHCH2CH:CH(CH2)4Me] at 50 mg/kg i.p. showed 157% increase in life span of mice transplanted with leukemia P-388 ceils.

IT 123824-76-0P 123824-79-3P 123824-80-6P

123880-12-6P 123880-13-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of, as neoplasm inhibitor)

Ι

RN 123824-76-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(2-hydroxyethyl)-, 5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, $[5R-(5\alpha,5a\alpha,8a\beta,9\alpha)]-(9CI)$ (CA INDEX NAME)

RN 123824-79-3 CAPLUS

CN [1,4'-Bipiperidine]-1'-carboxylic acid, 5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, [5R-(5 α ,5a α ,8a β ,9 α)]- (9CI) (CA INDEX NAME)

RN 123824-80-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(1,3-benzodioxol-5-ylmethyl)-, 5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester, [5R-(5 α ,5a α ,8a β ,9.alph a.)]- (9CI) (CA INDEX NAME)

RN 123880-12-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(2-hydroxyethyl)-, 5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl) furo[3',4':6,7]naphtho[2,3-d]-1,3-dioxol-5-yl ester, $[5S-(5\alpha,5a\beta,8a\alpha,9\beta)]-(9CI)$ (CA INDEX NAME)

RN 123880-13-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(1,3-benzodioxol-5-ylmethyl)-, 5,5a,6,8,8a,9-hexahydro-8-oxo-9-(3,4,5-trimethoxyphenyl)furo[3',4':6,7]nap htho[2,3-d]-1,3-dioxol-5-yl ester, [5S-(5α,5aβ,8aα,9.beta.)]- (9CI) (CA INDEX NAME)

L9 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1958:22209 CAPLUS Full-text

52:22209 CAPLOS <u>FUIT-LEXT</u>

DOCUMENT NUMBER:

52:4023e-g

ORIGINAL REFERENCE NO.: TITLE:

Effects of a podophyllotoxin derivative on tissue

culture systems in which human cancer invades normal

tissue '

AUTHOR(S):

Leighton, Joseph; Kline, Ira; Belkin, Morris; Orr,

Henry C.

CORPORATE SOURCE:

Natl. Cancer Inst., Bethesda, MD

SOURCE:

Cancer Research (1957), 17, 336-44

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

AB Acetylpodophyllotoxin- ω -pyridinium chloride (NCI 3022) (I), in concentration of 1 γ /ml., applied for 6 hrs. to sponge-matrix tissue culture systems in which cells derived from a carcinoma (Strain HeLa) had invaded normal tissue, produced complete metaphase arrest in both normal and tumor cells; removal of I after 6 hrs. was followed by almost complete disappearance of its effect in 18 hrs. When a dose of 1 γ /ml. was given on alternate days for 4 weeks, the effect on tumor cells was much more severe than on normal cells.

IT 122146-76-3, Podophyllotoxin, ester with 1-

(carboxymethyl)pyridinium chloride

(effect on cancer cells)

RN 122146-76-3 CAPLUS

L9 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1957:36019 CAPLUS Full-text

DOCUMENT NUMBER: 51:36019 ORIGINAL REFERENCE NO.: 51:6870b-e

TITLE: Effect of various drugs on the tumor-necrotizing

activity of several chemical agents in mice

AUTHOR(S): Pradhan, Sachindra N.; Achinstein, Betty; Shear,

Murray J.

CORPORATE SOURCE: Natl. Cancer Inst., Bethesda, MD

SOURCE: Cancer Research (1956), 16, 1062-8

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

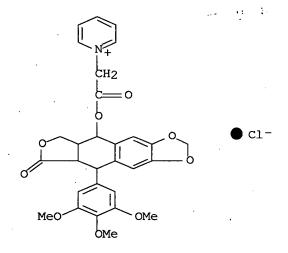
AΒ In mice bearing Sarcoma 37, the tumor-necrotizing potency of the bacterial polysaccharide from Serratia marcescens was reduced by dibenamine, dibenzyline, priscoline, cortisone, and urethan, and not by regitine, dihydroergotamine, pentobarbital sodium, or phenobarbital sodium. The tumornecrotizing potency of pitressin was inhibited by atropine, dibenzamine, dibenzylamine, and phenobarbital sodium, not by cortisone or pentobarbital sodium. Tumor necrosis induced by serotonin was inhibited by dibenzyline, dibenamine, and priscoline, not by the other drugs. Tumor necrosis by amphetamine was inhibited by dibenzyline and urethan. Tumor necrosis by histamine was inhibited by atropine, dibenzamine, dibenzyline, and pentobarbital sodium, not by cortisone or phenobarbital sodium. Tumor necrosis by acetylpodophyllotoxin-o-pyridinium chloride was not affected by any of the compds. used. The lethal toxicity of amphetamine was increased by

IT 122146-76-3, Podophyllotoxin, ester with 1-(carboxymethyl)pyridinium chloride (effect on tumor-necrotizing compds.)

RN 122146-76-3 CAPLUS

atropine.

CN 1-(Carboxymethyl)pyridinium chloride, ester with podophyllotoxin (6CI) (CA INDEX NAME)



L9 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1956:89760 CAPLUS Full-text

DOCUMENT NUMBER:

50:89760

ORIGINAL REFERENCE NO.:

50:16920g-i,16921a

TITLE:

Enzyme changes induced in normal and malignant tissues with chemical agents. VII. Effect on hydrolytic and synthetic enzymes of diphosphopyridine nucleotide in

sarcoma 37

AUTHOR(S):

Waravdekar, V. S.; Powers, O. H.; Leiter, J.

CORPORATE SOURCE:

Natl. Cancer Inst., Bethesda, MD

SOURCE:

Journal of the National Cancer Institute (1940-1978)

(1956), 17, 145-54

CODEN: JNCIAM; ISSN: 0027-8874

DOCUMENT TYPE:

Journal LANGUAGE: Unavailable

AB cf. C.A. 50, 11501e. The diphosphopyridine nucleotidase ((DPN)-ase) and DPNpyrophosphatase activities of various transplanted tumors in mice were determined The DPN-ase and DPN-pyrophosphatase activity of homogenates of sarcoma 37 and of liver from tumor-bearing mice receiving injections of 20 γ/g . of acetylpodophyllotoxin- ω -pyridinium chloride showed rather small changes in enzyme activity in comparison with those in similar tissues from animals not treated with the drug. The ability of tumor homogenates from the treated animals to synthesize DPN was markedly reduced, while the capacity for synthesis of DPN from nicotinamide mononucleotide by the homogenates of livers from these animals increased in proportion to the damage induced in the tumors. Disruption of liver cells from nontumor-bearing mice and of tumor cells by phys. means resulted in a 50% loss in ability of the enzyme in these tissues to synthesize DPN. Liver homogenates from tumor-bearing mice showed approx. 50% less activity for synthesis of DPN than did the homogenates of the livers from nontumor-bearing mice.

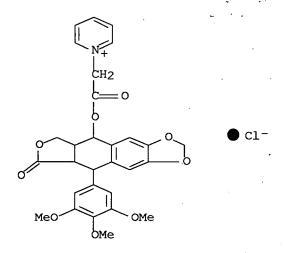
ΤТ 122146-76-3, Podophyllotoxin, ester with 1-

(carboxymethyl)pyridinium chloride

(effect on diphosphopyridinenucleotidase and diphosphopyridinepyrophosphatase in neoplasms)

RN 122146-76-3 CAPLUS

CN 1-(Carboxymethyl)pyridinium chloride, ester with podophyllotoxin (6CI) (CA INDEX NAME)



L9 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1956:61233 CAPLUS Full-text

DOCUMENT NUMBER:

50:61233

ORIGINAL REFERENCE NO.:

50:11501b-е

TITLE:

Enzyme changes induced in normal and malignant tissues

with chemical agents. VI. Effect of

acetylpodophyllotoxin-ω-pyridinium chloride on

malic oxidase and isocitric oxidase systems of sarcoma

37

AUTHOR(S):

Waravdekar, V. S.; Powers, O.; Leiter, J.

CORPORATE SOURCE:

Natl. Cancer Inst., Bethesda, MD

SOURCE:

Journal of the National Cancer Institute (1940-1978)

(1956), 16, 1443-52

CODEN: JNCIAM; ISSN: 0027-8874

DOCUMENT TYPE:

LANGUAGE:

Unavailable

Journal

AB cf. C.A. 49, 14191c. Homogenates of sarcoma 37 from mice that had received a single subcutaneous injection of 20 γ of acetylpodophyllotoxin- ω -pyridinium chloride (I)/g. showed a marked decrease in malic oxidase activity. hrs. after injection most of the activity was lost, whereas malic dehydrogenase activity was scarcely affected. In the tumor, other enzyme systems closely associated with the malic oxidase system, such as maliccytochrome c reductase, diphosphopyridine nucleotide (DPN)-cytochrome c reductase, and reduced DPH (DPNH) oxidase, were equally affected by I. Addition of cytochrome c enhanced the DPNH-oxidase activity of both treated and untreated tissues in proportion to their respective activities; addition of DPN increased the malic-cytochrome c reductase activity of the tissues. Oxidation of d-isocitrate by the homogenates of tumors from I-treated animals was markedly lowered but isocitric dehydrogenase was unaffected. Other components of this system, such as triphosphopyridine nucleotide- cytochrome c reductase activity of the treated tumor, also showed marked decrease in activity. The effects of I on the specific oxidase systems (succinic, malic, and isocitric) could be accounted for by the action on the cytochrome system.

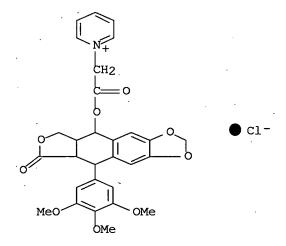
IT 122146-76-3, Podophyllotoxin, ester with 1-

(carboxymethyl)pyridinium chloride

(effect on enzymes in cancerous tissue)

RN 122146-76-3 CAPLUS

CN 1-(Carboxymethyl)pyridinium chloride, ester with podophyllotoxin (6CI) (CA INDEX NAME)



ANSWER 17 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1955:74734 CAPLUS Full-text

DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.:

49:74734

49:14191e-h

TITLE:

Enzyme changes induced in normal and malignant tissues

with chemical agents. V. Effect of

acetylpodophyllotoxin-ω-pyridiniumchloride on

uricase, adenosine deaminase, nucleoside

phosphorylase, and glutamic dehydrogenase activities

Waravdekar, V. S.; Paradis, Anita D.; Leiter, J.

AUTHOR(S): CORPORATE SOURCE:

Natl. Cancer Inst., Bethesda, MD

SOURCE:

Journal of the National Cancer Institute (1940-1978)

(1955), 16, 99–105

CODEN: JNCIAM; ISSN: 0027-8874

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

AΒ Homogenates of sarcoma 37 from mice injected with 20 γ /g. of acetylpodophyllotoxin-w-pyridinium chloride showed a marked decrease in the mitochondrial enzyme, uricase. Only 25% of the uricase activity of control tissue was observed in the tumor tissue from animals killed 6 h. after the injection. Adenosine deaminase and nucleoside phosphorylase, 2 enzymes in the soluble fraction of the cell, were only slightly affected during the same time interval. Smaller decreases were also observed in the dehydrogenase activity in homogenates of hepatoma 129 from treated animals as compared with homogenates from untreated animals, even after the homogenates were forced through a tissue press at 20,000 lb. sq. in. The percentage of residual activity in lumor homogenates from mice 24 h. after treatment with acetylpodophyllin-o-pyridinium chloride was: cytochrome oxidase, 66; succinic oxidase, 2; uricase, 2; glutamic dehydrogenase, 46. The glutamic dehydrogenase activity of a variety of tumors in untreated animals was determined Values for glutamic dehydrogenase in tumors other than hepatoma were 1/12 to 1/30 that of liver; hepatoma showed an activity about 3-7 times that of other tumors. The relation between the biochem. changes and the structural integrity of some cell particulates is discussed.

ΙT 122146-76-3, Podophyllotoxin, ester with 1-(carboxymethyl)pyridinium chloride

(enzyme changes induced by)

RN 122146-76-3 CAPLUS

(enzyme changes produced by

L9 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1955:74733 CAPLUS Full-text

DOCUMENT NUMBER:

49:74733 49:14191b-e

ORIGINAL REFERENCE NO.: TITLE:

Enzyme changes induced in normal and malignant tissues

with chemical agents. IV. Effect of α -peltatin on glucose utilization by sarcoma 37 and on the adenosinetriphosphatase, hexokinase, aldolase, and

pyridine nucleotide levels of sarcoma 37

AUTHOR(S):

Waravdekar, V. S.; Paradis, Anita D.; Leiter, J.

CORPORATE SOURCE:

Natl. Cancer Inst., Bethesda, MD

SOURCE:

Journal of the National Cancer Institute (1940-1978)

(1955), 16, 31-9

CODEN: JNCIAM; ISSN: 0027-8874

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

after a single subcutaneous dose of $20~\gamma/g$. of α -peltatin showed about 40% decreased ability to utilize glucose anaerobically in comparison with homogenates from untreated mice. With increasing diphosphopyridine nucleotide (DPN) concentration in the medium, α -peltatin-treated tumor homogenates showed an increased ability to utilize glucose, reaching a maximum at a DPN concentration of 0.006M. Similar increases in DFN levels did not increase the ability of control tumor to utilize more glucose over that observed with 0.00016M DPN in the medium. At a DPN concentration of 0.006M the glucose uptake by control and treated tumor was the same. The same dose of α -peltatin produced a marked drop in DPN level of sarcoma 37 soon after administration. Only small changes in adenosinetriphosphatase, aldolase, and hexokinase activities were observed during the period (4-6 hrs.) in which the glucose utilization and DPN level exhibited marked decreases.

IT 122146-76-3, Pyridinium, 1-(carboxymethyl)-, chloride, ester with podophyllotoxin

(enzyme changes produced by)

RN 122146-76-3 CAPLUS

L9 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1954:15943 CAPLUS Full-text

DOCUMENT NUMBER: 48:15943
ORIGINAL REFERENCE NO.: 48:2922g-i

TITLE: Enzyme changes induced in normal and malignant tissues

with chemical agents. III. Effect of

acetylpodophyllotoxin-ω-pyridinium chloride on cytochrome oxidase, cytochrome c, succinoxidase, succinic dehydrogenase, and respiration of sarcoma 37

AUTHOR(S): Waravdekar, V. S.; Paradis, Anita D.; Leiter, J.

CORPORATE SOURCE: Natl. Cancer Inst., Bethesda, MD

SOURCE: Journal of the National Cancer Institute (1940-1978)

(1953), 14, 585-92

CODEN: JNCIAM; ISSN: 0027-8874

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB cf. C.A. 47, 1852c, 11555f. A single subcutaneous injection of 20 γ/g . of acetylpodophyllotoxin- ω -pyridinium chloride (I) in mice bearing sarcoma 37 produced a marked drop in cytochrome oxidase activity, cytochrome c, and succinoxidase (II) activity of liver homogenates, and a marked decrease in respiration of tumor slices. Even a lethal dose of I only slightly reduced the succinic dehydrogenase activity. In liver, kidney, spleen, and lung of tumor-bearing mice treated with a maximum tolerated dose (80 γ/g .) of I, a much smaller percentage decrease in II activity was observed than in tumor tissue. In vitro incubation of tumor slices with I, podophyllotoxin, or colchicine in concns. up to 250 γ/cc . produced smaller changes in II activity and respiration than those observed after the same interval following treatment in vivo.

IT 122146-76-3, Podophyllotoxin, ester with 1 (carboxymethyl)pyridinium chloride
 (enzyme changes produced by)

RN 122146-76-3 CAPLUS

CN 1-(Carboxymethyl)pyridinium chloride, ester with podophyllotoxin (6CI) (CA INDEX NAME)

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L4 52 S E1-E52

L5 87 S L1 SSS FULL

L6 STRUCTURE UPLOADED

L7 80 S L6 FULL SUB=L5

L8 8 S L4 AND L5

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